OPENMC IS COOL

Day 1 – Monte Carlo and OpenMC Overview

GOALS FOR TODAY

- Monte Carlo (Stochastic Methods)
- Constructive Solid Geometry (CSG)
- OpenMC Particle Transport
- Active cycles/particles
- keff calculations
- Shannon Entropy/inactive cycles
- continuous energy, and multi group x-sections
- Thermal Scattering Laws
- P tables (unresolved resonance range)
- Flux and other tallies
- Depletion
- Parallelization
- Applications of Monte Carlo Methods

ONE OF YOUR BEST RESOURCES WILL BE THE OPENMC DOCUMENTATION FOR BOTH METHODOLOGY AND SYNTAX QUESTIONS:

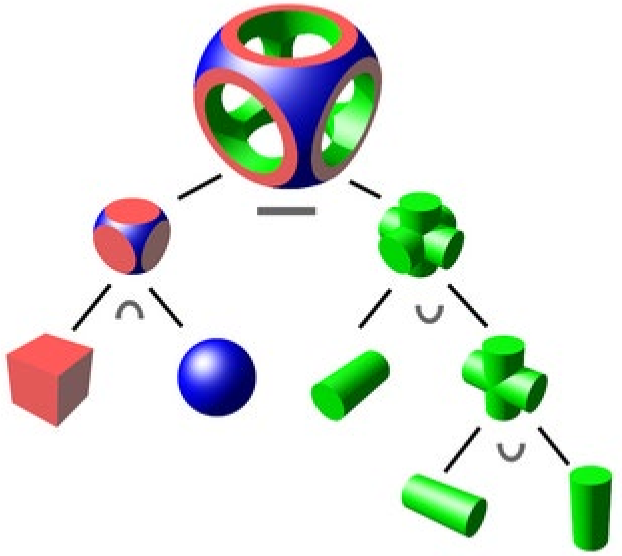
[HTTPS://DOCS.OPENMC.ORG/EN/STABLE/](https://docs.openmc.org/en/stable/)

MONTE CARLO (STOCHASTIC METHODS)

- Stochastic Risk Stats Calculation
  - [Run though the Notebook with the Risk game stats calculation using Monte Carlo]
  - Use known probabilities to calculate a value without actually doing any real math
  - Differentiate between iterations and trials
  - Results include stdev
  - How stdev and time scale

CSG (CONSTRUCTIVE SOLID GEOMETRY)

- The creation of complex shapes using the intersection of simple shapes
- We use second order surfaces
- This gives Monte Carlo Calculations a "general geometry"



https://en.wikipedia.org/wiki/Constructive_solid_geometry

OPENMC PARTICLE TRANSPORT

$$\ell = -\frac{\ln \xi}{\Sigma_t}$$

- To begin, particles are set with initial location, directions, and energy.
- Based on the material the particle is in, a path length is calculated.
- At the end of the path length, if the particle has not crossed a surface, then an interaction occurs. Which particular interaction depends on how big the cross sections are for each particular interaction (ie. fission, cross section, absorption, scattering, etc.). The data for cross section magnitude for each isotope is in the fundamental nuclear cross section data that we downloaded in week 1
- After an interaction occurs, a tally is made to record what happened. If the particle wasn't destroyed (ie. an absorption interaction occurred), then a new direction, energy, and path length are calculated, and the particle travels again. This is done until the particle is destroyed
- Millions of particles will be simulated, and the tallies will give information needed to calculate what is happening in the system.

ACTIVE CYCLES/PARTICLES

- Each "cycle" is the simulation of the lifetime of a number of particles. Batch and generation are also terms used for cycle
- When you set up the simulation, you will specify a number of cycles, and a number of particles per cycle.
- Cycles exist because this is a "generational" process. When fissions occur, the location of fission sites is noted in the code, and the fission neutron is recorded (along with its energy, direction, and now a weight) which contributes to the next generation/cycle
- For example, when you run a simulation, you might use 100 active cycles and 1 million particles per cycle

KEFF CALCULATIONS

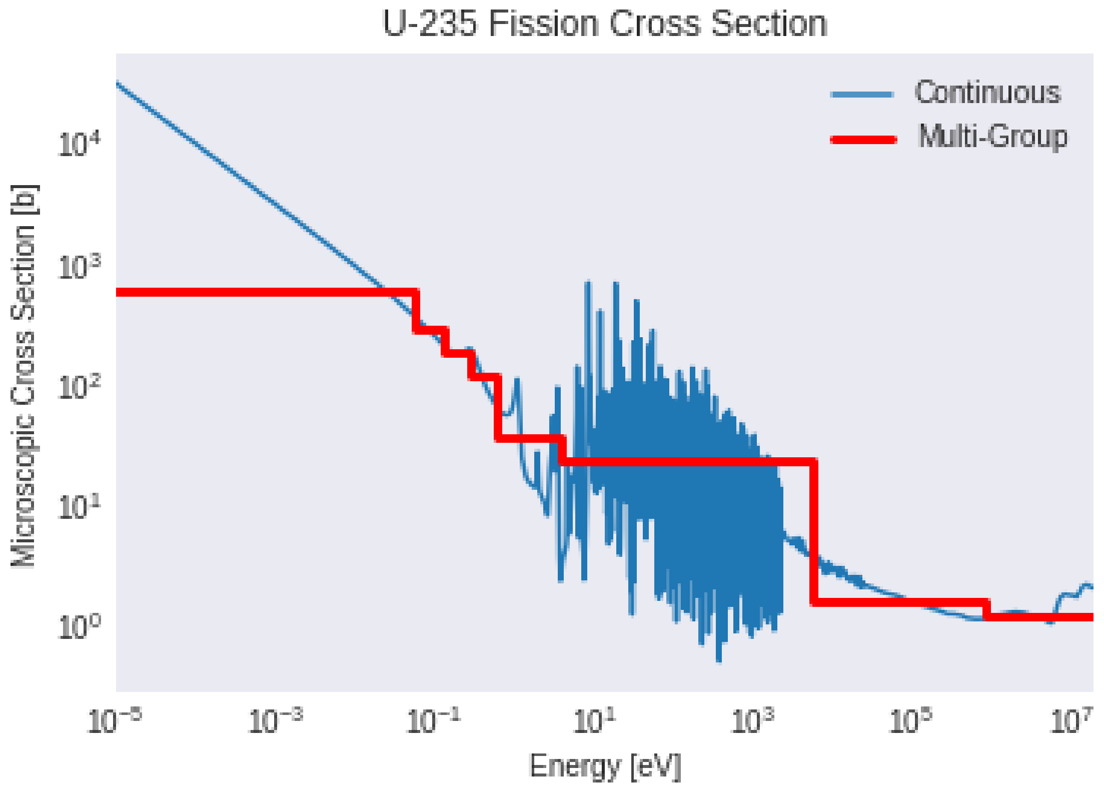
- keff is calculated using the Method of Successive Generations (see OpenMC Documentation for more details, and literature)
- keff can be thought of as the number of particles in the a new generation / the number of particles in the previous generation
- We run a number of generations, and the keff values converge to a value at some point, and we can take an average of the "good" keff values for our solution of what keff is

SHANNON ENTROPY & INACTIVE CYCLES

- I say "good" keff calculations, because as noted before, you have to have an initial position, energy, and direction for the particles, and whatever we guess for the initial conditions, we will be wrong.
- Fortunately, we know that with each generation, the particles will spread out to reflect an accurate distribution, or in other words, the distribution of the particles will converge to the correct answer.
- The way that we measure if our solution is "converged" is with Shannon Entropy which is really just a measure of how much the distribution of sites is changing
- Once Shannon Entropy converges, we can be pretty confident that our keff values have converged
- Inactive cycles are cycles that we run where the particles are simulated like norma, but the data doesn't contribute to our final answer.
- When running a simulation, you want to set enough inactive cycles for Shannon Entropy to converge. For example, you might run 50 inactive cycles, 100 active cycles, and 1 million particles per cycle.

CONTINUOUS ENERGY, AND MULTI GROUP X-SECTIONS

- Constant cross sections across energy bins
- Most (determenistic) neutronic codes run with multigroup cross section data
- Monte Carlo can run with either MG (multi group) or CE (continuous energy) cross section data
- Monte Carlo can also be used to generate MG cross section data



https://github.com/openmc-dev/openmc/wiki/Example-Jupyter-Notebooks

>>Multigroup Cross Section Generation Part II: Advanced Features

THERMAL SCATTERING LAWS (TSLs)

- Thermal (low energy end of spectrum) interacts with a bond or a lattice instead of an individual atom (ie an H-O bond in water)
- (Also called S(α, β) tables)
- ie. In order to simulate water in our code, we need to not only specify how many H atoms and how many O atoms are present, but we need to also specify that the O and H atoms are bonded.
- Examples of TSLs that can be applied in OpenMC
  - 'c_H_in_H2O" (continuous energy, H in H2O)
  - "c_D_in_D2O" (deuterium in heavy water)
  - "c_C_in_graphite" (carbon in graphite)
  - "c_Be_in_BeO" (Beryllium in Beryllium Oxide)
  - "c_O_in_BeO" (Oxygen in Beryllium Oxide)
  - etc.

P TABLES (UNRESOLVED RESONANCE RANGE)

- URR is from neutron energies of about 100 keV to 2 MeV (for things such as U238)
- In the URR, we have a hard time characterizing x-section data at the intermediate range of neutron energies (peaks are very closely spaced and hard to characterize)
- We can not resolve the resonances with our measurement techniques in this region because they are so close together
- Instead we use probability tables to get statistical descriptions of this range (ie. mean level spacing, or mean resonance width)
- (note: as users we aren't going to be doing anything with ptables, but you should know that this is how Monte Carlo methods deal with those particular neutron energies)

FLUX TALLY (AND OTHER TALLIES)

- A tally is pretty much a count of how many times something happened
- The most basic tally is flux (number of neutrons passing through a unit area)
- We can also tally reaction rates for any particular reaction
- Common tallies to keep track of:
  - Reaction Rate
  - Absorption Rate
  - Fission Rate
  - kappa-fission (recoverable energy production rate due to fission)

FLUX TALLY (AND OTHER TALLIES)

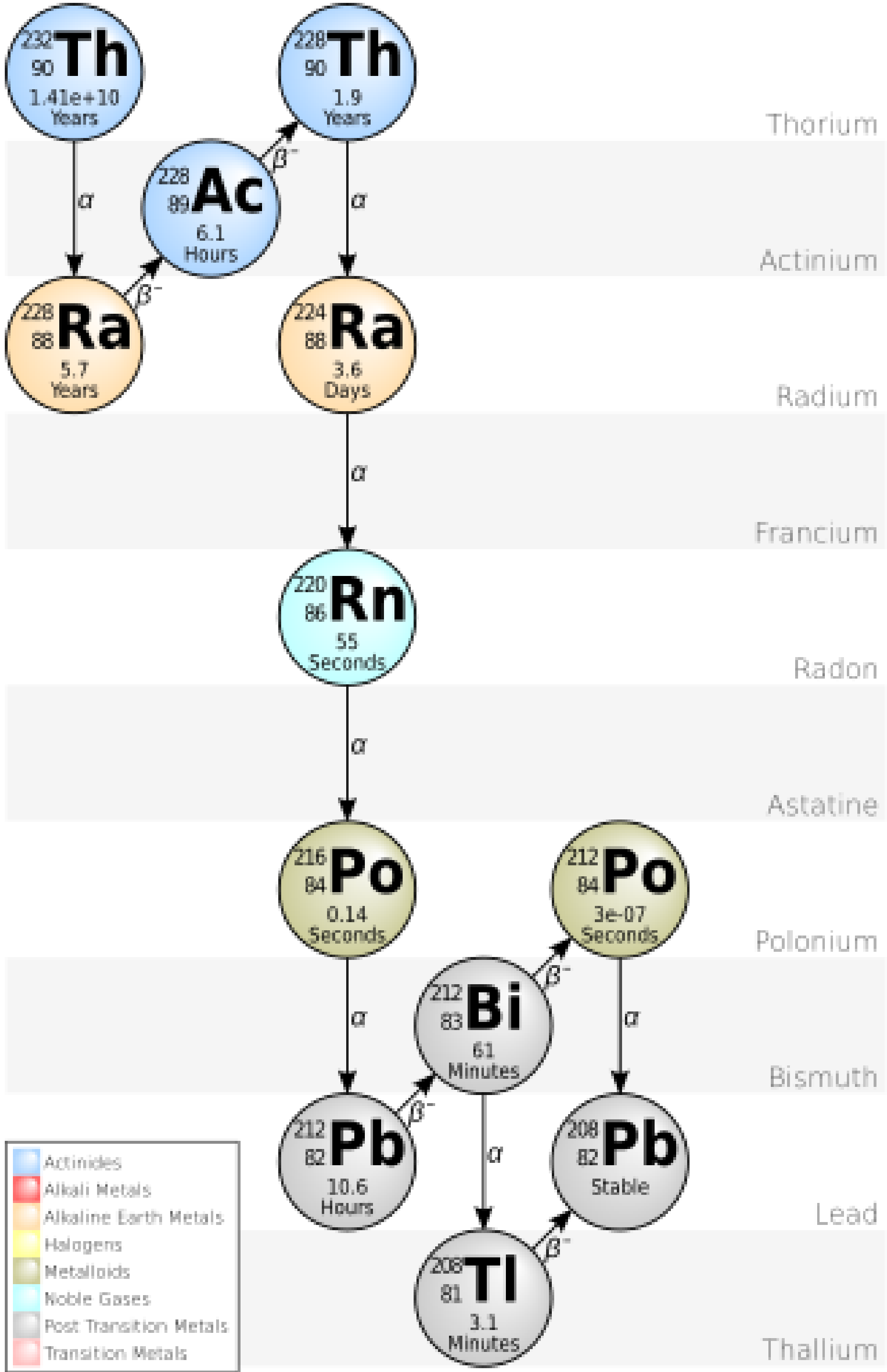
$$X = \underbrace{\int d\mathbf{r} \int d\mathbf{\Omega} \int dE}_{\text{filters}} \underbrace{f(\mathbf{r}, \mathbf{\Omega}, E)}_{\text{scores}} \psi(\mathbf{r}, \mathbf{\Omega}, E)$$

r	Position in space — typically a point in 3D coordinates (x, y, z) or a volume region.
Ω	Neutron direction — unit vector representing the neutron's travel direction (angle in 3D space).
E	Neutron energy.
dr	Differential spatial volume element.
dΩ	Differential solid angle element (direction space).
dE	Differential energy element.

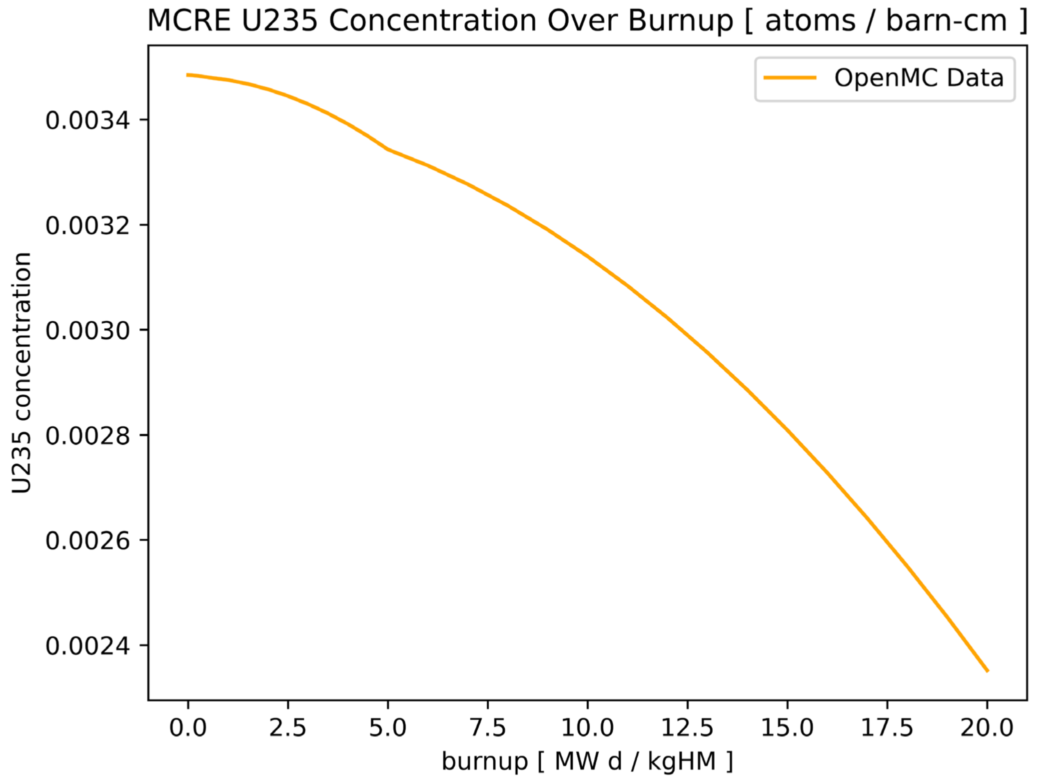
ψ(r,Ω,E)	Neutron angular flux — neutron flow rate through space, direction, and energy. It represents how many neutrons exist at that position, going in that direction, with that energy.
f(r,Ω,E)	**Score function** — describes what quantity you want to measure (e.g., flux, reaction rate, absorption, fission).
X	Final tally result — the quantity being measured (like total flux, absorption rate, dose, etc.).

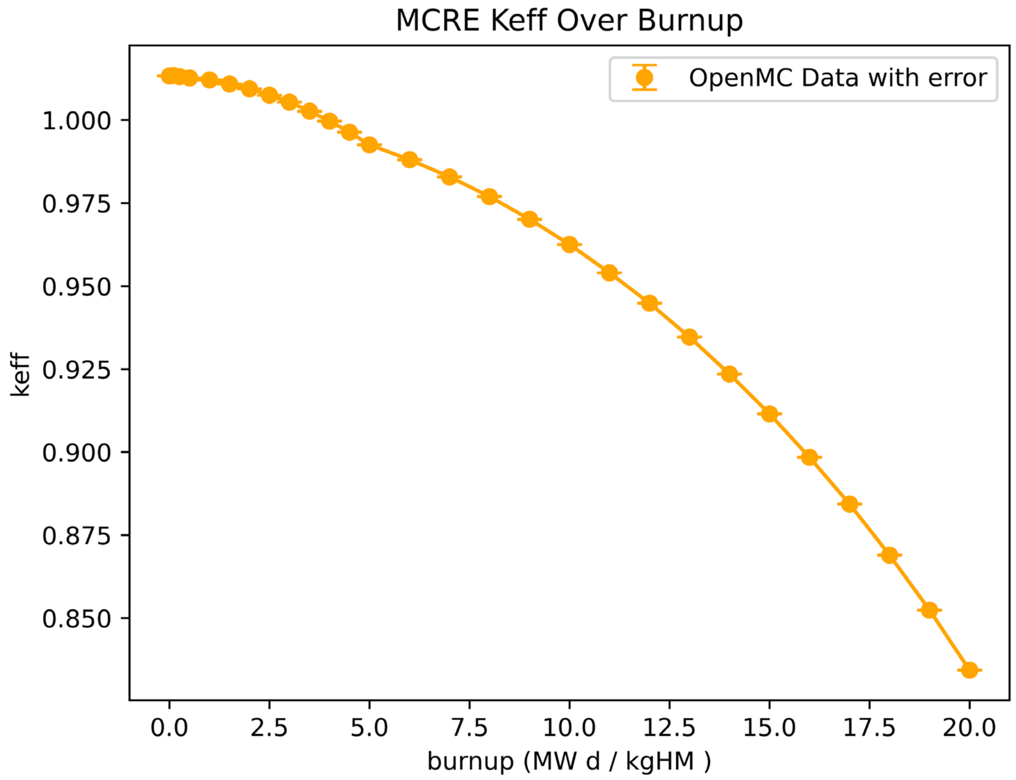
DEPLETION

- k-eigenvalue calculations calculate the data at a given point
- A depletion calculation (also called burnup calculation) will calculate nuclide densities within a material over time (ie. what is going to be in my reactor in 6 months? a year? etc.?)
- A depletion is a repetition of calculating your transport equation and the transmutation equations. There are different methods for optimizing these calculations
- The concentration of nuclides is calculated using data from decay chains (our OPENMC_CHAIN_FILE data that we installed in week 1 along with cross section data)
- Bateman/Transmutation equations are used to solve for the change in the amount of each nuclide present over time

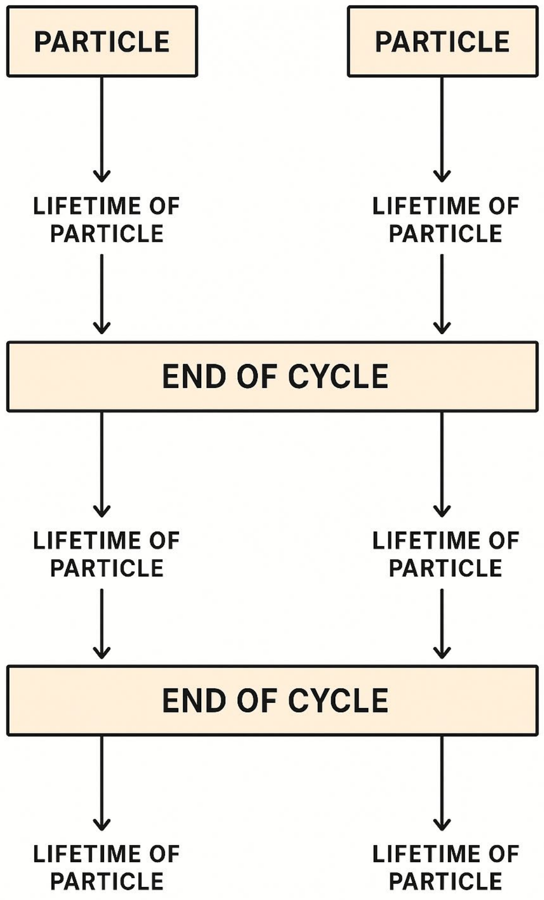


DEPLETION (SOME EXAMPLE DATA OUTPUT)





PARALLELIZATION



- In each generation, the lifetime of every particle is independent of every other particle
- This is good for parallel computing because a significant amount of computation is used in particle tracking and x-section look up
- In order to calculate the tallies at the end of each generation, however, the data from each particle lifetime is required
- Thus parallelization is done as follows:
  - Geometry and nuclear data are loaded once and replicated on each process/thread
  - The first cycle begins
  - Particles lives/histories are tracked on separate threads
  - At the end of the cycle, the threads communicate and tally data is computed
  - The next cycle begins

APPLICATIONS OF MONTE CARLO METHODS - OPENMC

Examples of actual things you could/would run in OpenMC

- Compute keff for a 17×17 PWR assembly with various enrichments
- Find radial power peaking factors in a full-core SMR model
- Simulate void coefficient for a BWR at different power/flow states
- Calculate dose rate behind a shielding wall
- Perform burnup calculation for a pin to 60 GWd/MTU and examine isotopic buildup
- Determine if a spent fuel cask is safely subcritical under flooding conditions
- Run a mesh tally to compute neutron flux along a reactor vessel wall
- Evaluate the reactivity worth of a control rod movement.
- Run an accident scenario, like cold-water reactivity insertion, by varying moderator temperature
- Generate multi-group cross section data for a deterministic core simulator

INSTALLATION TROUBLESHOOTING. ANY QUESTIONS / CONCERNS?

OTHER EXAMPLE APPLICATIONS (IF EXTRA TIME)

APPLICATIONS OF MONTE CARLO METHODS - HIGH LEVEL

- Nuclear Engineering (Neutron & Photon Transport)
- Detector design and calibration
- Cosmic ray and astrophysics simulations
- Modeling of electron/photon transport in materials
- Computational Chemistry
- Fusion reactor design
- Radiation therapy dose calculations
- Imaging physics (PET/SPECT)

(Not all can be done with OpenMC, just Monte Carlo Methods)

APPLICATIONS OF MONTE CARLO METHODS - NEUTRONIC MODELING

- Common Monte Carlo Codes
  - MCNP (Oak Ridge National Lab)
  - Serpent (National Lab in Finland)
  - OpenMC (Open source, Originated at MIT, contributions from labs)
  - SCALE (Oak Ridge National Lab)

APPLICATIONS OF MONTE CARLO METHODS - OPENMC

- Reactor Core Physics - model a reactor core and compute:
    - multiplication factor (k-eff)
    - Power distribution (axial, radial)
    - Fission rate or reaction rate maps
    - Flux distribution
    - Component reactivity comparisons
    - Fuel depletion over burnup

- Fuel Assembly or Pin-Cell Calculations
    - Infinite multiplication factor (k-inf)
    - Doppler temperature coefficients
    - Moderator temperature/void coefficients
    - Effects of fuel enrichment or burnable absorbers

APPLICATIONS OF MONTE CARLO METHODS - OPENMC

- Criticality Safety Evaluations - keff + uncertainty, sensitivity to material/geometry variations
  - Fresh fuel storage racks
  - Spent fuel pools
  - Transport containers (dry casks, railcar transports)
  - Chemical processing tanks with fissile solutions

- Radiation Shielding and Dose Calculation
  - Dose rate
  - Shutdown dose calculations

- Depletion / Burnup Studies
  - Fuel isotopic evolution
  - Burnup-dependent reactivity changes
  - Actinide buildup and fission product poisoning
  - Decay heat estimation

APPLICATIONS OF MONTE CARLO METHODS - OPENMC

- Coupling with Thermal-Hydraulics or Fuel Performance Codes
- Experiment Benchmarking
- Waste classification studies
- Detector design
- Neutron scattering experiments
- Neutron imaging and shielding problems